



Product Safety and Regulatory Affairs

201-14960

December 22, 2003

Marianne L. Horinko
Acting Administrator
U.S. Environmental Protection Agency
P.O. Box 1473
Merrifield, VA 22116

Attn: Chemical Right To-Know Program

Dear Administrator Horinko,

Crompton Corporation is submitting the enclosed Robust Summary and Test Plan for the following chemical:

Eicosenoic acid, methyl ester, (Z)- (CAS RN: 76899-35-9)

If you have any questions, please contact me at 203-573-3390 or e-mail to mark_Thomson@cromptoncorp.com

Sincerely,

Dr. Mark A. Thomson
Manager, Toxicology & International Product Registration
Crompton Corporation
Middlebury, CT 06749
USA

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**HIGH PRODUCTION VOLUME (HPV)
CHEMICAL CHALLENGE PROGRAM**

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TEST PLAN

For

Eicosenoic acid, methyl ester, (Z)-

CAS No. 76899-35-9

Submitted to the US EPA

BY

Crompton Corporation.

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Test Plan for Eicosenoic acid, methyl ester, (Z)-

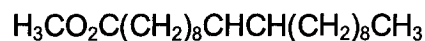
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1. General Information

1.1 CAS Number: 76899-35-9

1.2 Molecular Weight: 324.55

1.3 Structure and formula: C₂₁H₄₀O₂



1.4 Introduction

The substance is used as ??????????

2. Review of Existing Data and Development of Test Plan

Crompton Corporation has undertaken a comprehensive evaluation of all relevant data on the SIDS endpoints of concern for the substance.

The availability of the data on the specific SIDS endpoints is summarized in Table 1. Table 1 also shows data gaps that will be filled by additional testing.

Table 1: Available adequate data and proposed testing on eicosenoic acid, methyl ester, (Z)-

CAS No. 76899-35-9	Information Available?	GLP	OECD Study?	Other Study?	Estimation Method?	Acceptable?	SIDS Testing required?
	Y/N	Y/N	Y/N	Y/N	Y/N	Y/N	Y/N
Physicochemical							
Melting Point	Y				Y	Y	N
Boiling Point	Y				Y	Y	N
Vapour Pressure	Y				Y	Y	N
Water Solubility	Y				Y	Y	N
Partition Coefficient (Kow)	Y				Y	Y	N
Environmental Fate							
Biodegradation	Y				Y	Y	N
Hydrolysis	Y				Y	Y	N
Photodegradation	Y				Y	Y	N
Transport and Distribution between Environmental Compartments	Y				Y	Y	N
Ecotoxicology							
Acute Fish	Y				Y	Y	N
Acute Daphnia	Y				Y	Y	N
Acute Algae	Y				Y	Y	N

Toxicology							
Acute Oral	N						Y
Repeat Dose toxicity	N						Y
Genetic toxicity – Gene mutation	N						Y
Genetic toxicity – Chromosome aberration	N						Y
Reproductive toxicity	N						Y
Developmental toxicity/teratogenicity	N						Y

A. Evaluation of Existing Physicochemical Data and Proposed Testing

1. Melting Point

The melting point was estimated to be 98.13°C using MPBPWIN v 1.40.

2. Boiling Point

The boiling point was estimated to be 375.8°C using MPBPWIN v 1.40.

3. Vapor Pressure

The vapor pressure was estimated to be 0.0000083 hPa at 25°C using MPBPWIN v 1.40.

4. Water Solubility

The water solubility is estimated to be 0.00018 mg/L at 25°C using WSKOW v 1.40.

5. Partition Coefficient

The Log Pow is estimated to be 9 using KOWWIN v 1.66.

Summary of Physicochemical Properties Testing: Existing data for melting point, boiling point, vapour pressure, partition coefficient and water solubility are considered to fill these endpoints adequately.

B. Evaluation of Existing Environmental Fate Data and Proposed Testing

1. Biodegradation

The biodegradability of the chemical has been estimated using Biowin v4.00 and the results indicate the chemical to be readily biodegradable.

2. Hydrolysis

The half life at pH 7 is estimated to be 7.28 years, and at pH 8 266 days using HYDROWIN v 1.67.

3. Photodegradation

The potential for photodegradation of the chemical has been estimated using the AOPWIN v1.90, and indicated atmospheric oxidation via OH radicals reaction with a half-life of 1.5 – 1.65 hours (cis- & trans- isomers, respectively).

4. Transport and Distribution between Environmental Compartments

An Epiwin Level III Fugacity Model calculation has been conducted and indicates distribution mainly to sediment and, to a lesser extent, soil for emissions of 1000 kg/hr simultaneously to air water and soil compartments.

Summary of Environmental Fate Testing: Existing data for photodegradation, biodegradation, hydrolysis and transport and distribution between environmental compartments are considered to fill these endpoints adequately.

C. Evaluation of Existing Ecotoxicity Data and Proposed Testing

1. Acute Toxicity to Fish

The LC₅₀ (96 h) was estimated to be 0.009 mg/L using ECOSAR v 0.99g. This is greater than the estimated limit of solubility of the substance.

2. Acute Toxicity to Daphnia

The EC₅₀ (48 h) was estimated to be 0.00011 mg/L using ECOSAR v 0.99g.

3. Acute Toxicity to Algae

The EC₅₀ (96 h) was estimated to be 0.0009 mg/L using ECOSAR v 0.99g. This is greater than the estimated limit of solubility of the substance.

Summary of Ecotoxicity Testing: The substance is estimated to be readily biodegradable and toxic to the aquatic environment close to, or above its limit of solubility. No further testing is proposed.

D. Evaluation of Existing Human Health Effects Data and Proposed Testing

1. Acute Oral Toxicity

An OECD 423 study will be conducted to fill this endpoint.

2. Repeat Dose Toxicity

An OECD 422 study will be conducted to fill this endpoint.

3. Genotoxicity

OECD 471 and 473 studies will be conducted to fill this endpoint.

4. Reproductive and Developmental Toxicity

An OECD 422 study will be conducted to fill this endpoint.

Summary of Human Health Effects Testing: No data exists for the human health effects endpoints. Appropriate studies will be conducted to fill these endpoints.

3. Evaluation of Data for Quality and Acceptability

The collected data were reviewed for quality and acceptability following the general US EPA guidance [2] and the systematic approach described by Klimisch et al [3]. These methods include consideration of the reliability, relevance and adequacy of the data in evaluating their usefulness for hazard assessment purposes. This scoring system was only applied to ecotoxicology and human health endpoint studies per EPA recommendation [4]. The codification described by Klimisch specifies four categories of reliability for describing data adequacy. These are:

- (1) **Reliable without restriction:** Includes studies or data complying with Good Laboratory Practice (GLP) procedures, or with valid and/or internationally accepted testing guidelines, or in which the test parameters are documented and comparable to these guidelines.
- (2) **Reliable with Restrictions:** Includes studies or data in which test parameters are documented but vary slightly from testing guidelines.
- (3) **Not Reliable:** Includes studies or data in which there are interferences, or that use non-relevant organisms or exposure routes, or which were carried out using unacceptable methods, or where documentation is insufficient.
- (4) **Not Assignable:** Includes studies or data in which insufficient detail is reported to assign a rating, e.g. listed in abstracts or secondary literature.

4. References

- [1] US EPA, EPI Suite Software, 2000
- [2] USEPA (1998). Guidance for Meeting the SIDS Requirements (The SIDS Guide). Guidance for the HPV Challenge Program. Dated 11/2/98.
- [3] Klimisch, H.-J., et al (1997). A Systematic Approach for Evaluating the Quality of Experimental Toxicological and Ecotoxicological Data. Regul. Toxicol. Pharmacol. 25:1-5
- [4] USEPA (1999). Determining the Adequacy of Existing Data. Guidance for the HPV Challenge Program. Draft dated 2/10/99.

201-14960B

I U C L I D

Data Set

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Robust Summaries

Existing Chemical	: ID: 76899-35-9
CAS Name	: Eicosenoic acid, methyl ester
CAS No.	: 76899-35-9
Molecular Formula	: C21H40O2
Molecular Weight	: 324.55
Status	:
Memo	: Eicosenoic acid, Crompton US HPV
Printing date	: 17.12.2003
Revision date	:
Date of last update	: 17.12.2003
Number of pages	: 1
Chapter (profile)	: Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	: Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	: Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2. Physico-Chemical Data

Id 76899-35-9

Date 17.12.2003

2.1 MELTING POINT

Value : 98.1 °C
Sublimation :
Method : other: Estimation using MPBPWIN v 1.40
Year : 2003
GLP :
Test substance : Chemical name: Eicosenoic acid, methyl ester (Z)-
CAS No.: 76899-35-9
Reliability : (2) valid with restrictions
17.12.2003 (1)

2.2 BOILING POINT

Value : 375.8 °C at
Decomposition :
Method : other: Estimation using MPBPWIN v1.40
Year : 2003
GLP :
Test substance : Chemical name: Eicosenoic acid, methyl ester (Z)-
CAS No.: 76899-35-9
Reliability : (2) valid with restrictions
17.12.2003 (1)

2.4 VAPOUR PRESSURE

Value : .0000083 hPa at °C
Decomposition :
Method : other (calculated): MPBPWIN v1.40
Year : 2003
GLP :
Test substance : Chemical name: Eicosenoic acid, methyl ester (Z)-
CAS No.: 76899-35-9
Reliability : (2) valid with restrictions
17.12.2003 (1)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : 9 at °C
pH value :
Method : other (calculated): KOWWIN v1.66
Year : 2003
GLP :
Test substance : Chemical name: Eicosenoic acid, methyl ester (Z)-
CAS No.: 76899-35-9
Reliability : (2) valid with restrictions
17.12.2003 (1)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water

2. Physico-Chemical Data

Id 76899-35-9

Date 17.12.2003

pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: WSKOW v1.40
Year : 2003
GLP :
Test substance : Chemical name: Eicosenoic acid, methyl ester (Z)-
CAS No.: 76899-35-9
Reliability : (2) valid with restrictions
17.12.2003

(1)

3. Environmental Fate and Pathways

Id 76899-35-9

Date 17.12.2003

3.1.1 PHOTODEGRADATION

Type : air
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 1500000 molecule/cm³
Rate constant : cm³/(molecule*sec)
Degradation : % after
Deg. product :
Method : other (calculated): AOP v1.90
Year : 2003
GLP :
Test substance : Chemical name: Eicosenoic acid, methyl ester (Z)-
CAS No.: 76899-35-9

Result : rate constant (cis-isomer) = 77.5E-12 cm³/molecule-sec
rate constant (trans-isomer) = 85.14E-12 cm³/molecule-sec

T1/2 (cis-isomer) = 1.655 hours
T1/2 (trans-isomer) = 1.507 hours

Reliability : (2) valid with restrictions
17.12.2003 (1)

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : at °C
t1/2 pH9 : at °C
Deg. product :
Method : other (calculated): HYDROWIN v1.67
Year : 2003
GLP :
Test substance : Chemical name: Eicosenoic acid, methyl ester (Z)-
CAS No.: 76899-35-9

Result : T1/2 (pH 8) = 266 days

T1/2 (pH 7) = 7.28 years

Reliability : (2) valid with restrictions
17.12.2003 (1)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media :
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: EPIWIN Level III Fugacity Model

3. Environmental Fate and Pathways

Id 76899-35-9

Date 17.12.2003

Test substance : Chemical name: Eicosenoic acid, methyl ester (Z)-
CAS No.: 76899-35-9

	Mass Amount (percent)	Half-life (hr)	Emissions (kg/hr)
Air	0.098	1.29	1000
Water	7.3	360	1000
Soil	28	360	1000
Sediment	64.6	1440	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.34E-12	981	18.3	32.7	0.609
Water	4.84E-11	261	136	8.71	4.52
Soil	1.39E-13	1000	0	33.4	0
Sediment	1.45E-11	579	24	19.3	0.802

Persistence time: 620 hr

Reaction time: 659 hr

Advection time: 10400 hr

Percent reacted: 94.1

Percent advected: 5.94

Half-lives (hr), (based upon Biowin (ultimate) and Aopwin):

Air: 1.291

Water: 360

Soil: 360

Sediment: 1440

Biowin estimate: 2.921 (weeks)

Advection times (hr):

Air: 100

Water: 1000

Sediment: 5E+4

17.12.2003

(1)

3.5 BIODEGRADATION

Type : aerobic
Inoculum :
Contact time :
Degradation : (±) % after
Result : readily biodegradable
Deg. product :
Method : other: Calculated using BIOWIN v4.00
Year : 2003
GLP :
Test substance : Chemical name: Eicosenoic acid, methyl ester (Z)-
CAS No.: 76899-35-9

Result : MITI Linear Biodegradation Probability = 0.894

MITI Non-linear Biodegradation Probability - 0.929

17.12.2003

(1)

4. Ecotoxicity

Id 76899-35-9

Date 17.12.2003

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : other: Estimation
Species :
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : .009
Method : other: Estimation using ECOSAR v0.99g
Year : 2003
GLP :
Test substance : Chemical name: Eicosenoic acid, methyl ester (Z)-
CAS No.: 76899-35-9

17.12.2003

(1)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : other: Estimation
Species : Daphnia sp. (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
EC50 : .00011
Method : other: Estimation using ECOSAR v0.99g
Year : 2003
GLP :
Test substance : Chemical name: Eicosenoic acid, methyl ester (Z)-
CAS No.: 76899-35-9

17.12.2003

(1)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species :
Endpoint : growth rate
Exposure period : 96 hour(s)
Unit : mg/l
EC50 : .0009
Method : other: Estimation using ECOSAR v0.99g
Year : 2003
GLP :
Test substance : Chemical name: Eicosenoic acid, methyl ester (Z)-
CAS No.: 76899-35-9

17.12.2003

(1)

5. Toxicity

Id 76899-35-9

Date 17.12.2003

5.1.1 ACUTE ORAL TOXICITY

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

9. References

Id 76899-35-9
Date 17.12.2003

- (1) US EPA, EPIWIN v3.10, EPI Suite Software, 2000